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Over the duration of the grant, several papers were written by Short, his collaborators and students on AFOSR issues related to the proposal outline. Those that list whole or partial suppport of the AFOR (F49620-00-1-0005) are given below. Copies of the publications listed are also included. Some highlights of the most recent work are also included.

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Analytical Modelling of Ignition of Condensed Energetic Materials, Pulsed Detonation Engines and Miniaturization of Explosive Systems: Final report

Mark Short & Scott Stewart

AFOSR F49620-00-1-0005

§1 Objectives

The proposal concerned several issues dealing with the modelling of ignition, combustion, detonation propagation and detonation failure in both condensed and gaseous energetic materials, with particular relevance to miniaturized explosive and propulsion systems, and to pulsed detonation engines.

§2 Personnel supported

Over the duration of the grant, two PIs (Short & Stewart) and several graduate students were supported at various stages. The graduate students were Mr. Dave Kessler (Short, US student), Mr. Yanning Liu (Short), Mr. Dongyao Wang (Short) and Mr. Aslan Kasimov (Stewart).

§3 Interactions/Transitions

The PIs have been coordinating their efforts with on-going research at Eglin AFB (Dr. Joe Foster, Dr. Dave Lambert), and with the DX division at Los National National Laboratory (Dr. John Bdzil, Dr. Larry Hill, Dr. Steve Son, Dr. Blaine Asay). Some interactions with Dr. Fred Schauer, head of the pulsed detonation engine experimental facility at Wright Patterson, have also occurred.

§4 Visitors

Dr. Gary Sharpe (Department of Mathematics, University of Manchester, UK) visited UIUC from August 17th 2001 to September 17th 2001 and for two weeks in September 2002. His visit was funded by the AFOSR grant, and collaborated with Short on some detonation ignition and failure problems. These visits have resulted in three publications (refs. 2, 4, 7 listed below), with two more currently in preparation.

§5 Research accomplishments of the PIs

- **§5(a) PI - Short**

Over the duration of the grant, several papers were written by Short, his collaborators and students on AFOSR issues related to the proposal outline. Those that list whole or partial support of the AFOSR (F49620-00-1-0005) are given below. Copies of the publications listed are also included. Some highlights of the most recent work are described below.

Papers 2, 7 and 10 represent a concerted effort to understand ignition mechanisms and transition to detonation that occur in hydrocarbon fuels, relevant to PDEs. In 2, we used a model reaction mechanism, that importantly, distinguishes between the lengths of induction and heat release zones. In the classical one-step model, a well-defined induction zone necessarily implies a thin fire (heat release) zone, or, alternatively, a finite fire zone leads to no well-defined induction zone. We find that such reaction mechanisms may have a dramatic effect on the sequence of steps leading to detonation, in particular, chain-branching mechanisms have a tendency to generate subsonic, rather than supersonic, waves immediately after ignition. Other aspects of transition to detonation have been explored in these papers.

We have also made some important advances in understanding the dynamics of detonation instability in chain-branching fuels (4,13) and also derived new propagation laws for steady curved detonations in such materials (6). In particular, we find a new level of complexity that isn't present for the standard one-step models, and, in some sense, calls into question the validity of one-step models in describing some detonation phenomena.

Over the duration of the grant, work has also begun into the dynamics of ignition and detonation in miniaturized explosive systems. These lead to a new class of physical problems in high-speed reactive flow, brought about by the introduction of finite Reynolds number processes due to the small scale. One-paper (5) describes an ignition event in a narrow channel where acoustic times are short, but Reynolds number effects can still be ignored. Work in this area carried out over the duration of the grant remains to be written up, and this project will proceed with the new AFOSR contract, directed towards to miniature propulsion applications.

A major issue regarding the performance and safety of propellant and explosive materials is the burning that takes place in micron-size (25-200 micron) cracks. Such cracks may occur due to aging, or as a result of an ignition transient, e.g. an initiator impact event. In addition, due to the narrowness of the cracks, burning in such geometries may occur in a highly oscillatory manner, leading to substantial pressure variations in the gas-phase dynamics. The papers (1,3,8) have examined the mechanisms behind such burning in model rectangular cracks, highlighting the role of edge-flame oscillations. In particular, paper 8 is the first to identify edge-flame oscillations in premixed materials. Paper 1 establishes conditions for which edge-flame oscillations may occur in a crack between fuel and oxidizer boundaries, even for unit Lewis numbers. This work is also relevant to the new research project on miniaturized propulsion systems.

Finally some work on the DNS of transition to detonation in PDEs will be finished and written up.

(1) M. Short & Y. Liu 2002 *Edge-flame oscillations for unity Lewis numbers in a non-premixed counterflow*, Combust. Theor. Modell., submitted.

(2) G.J. Sharpe & M. Short 2002 *Shock induced ignition of thermally sensitive explosives*, IMA J. Appl. Math., submitted

(3) M. Short & Y. Liu 2002 *Instability and extinction of premixed flames in counterflows and thin channels*, Phys. Fluids, submitted.

(4) M. Short & G.J. Sharpe 2003 *Pulsating detonations for two-step reactions: theory and numerics*, Combust. Theory. Modell., accepted.

(5) A.K. Kapila & M. Short 2003 *Nondiffusive hot spot in a confined narrow domain*, J. Eng. Math. **45** 335-366.

(6) M. Short & J.B. Bdzil 2003 *Propagation laws for steady curved detonations with chain-branching kinetics*, J. Fluid Mech. **479** 39–64.

(7) G.J. Sharpe & M. Short 2003 *Detonation ignition from a temperature gradient for a two-step chain-branching kinetics model*, J. Fluid Mech. **476** 267–292.

(8) Y. Liu & M. Short 2002 *Premixed edge-flame oscillations in a rectangular channel with side-wall mass injection*, Combust. Theory Modell. **6** 607–623.

(9) M. Short & P.A. Blythe 2002 *Structure and stability of weak-heat-release detonations for finite Mach numbers*. Proc. Roy. Soc. Lond. A **458** 1795–1807.

(10) M. Short & J.W. Dold 2002 *Weak detonations and their role in transition to strong detonation*. Combust. Theory. Modell. **6** 279–296.

(11) M. Short, J.D. Buckmaster & S. Kochevets 2001 *Edge-flames and sublimit hydrogen combustion*, Combust. Flame. **125** 893–905.

(12) M. Short & D. Wang 2001 *On the dynamics of pulsating detonations*, Combust. Theory. Model. **5** 343–352.

(13) M. Short 2001 *A nonlinear evolution equation for pulsating Chapman-Jouguet detonations with chain-branching kinetics*. J. Fluid. Mech. **430** 381-400.

(14) S. Balachandar, J.D. Buckmaster & M. Short 2001 *The generation of axial vorticity in solid-propellant rocket-motor flows*. J. Fluid. Mech. **429** 283–305.

(15) M. Short 2000 *The power of distinguished limits: A comment on "On the two-dimensional instability of square-wave detonations" [CTM 2, 297 (1999)]*, Combust. Theory & Model. **4** 211-216.

(16) M. Short, A.K. Kapila & J.J. Quirk, 1999 *The chemical gas-dynamic mechanisms of pulsating detonation wave instability*. Phil. Trans. Roy. Soc. Lond. A. **357** 3621–3628.

(17) J.D. Buckmaster & M. Short, 1999, *Cellular Instabilities, Sub-Limit Structures and Edge-Flames in Premixed Counterflows*. Combust. Theory Modell. **3** 199–214.

(18) M. Short & D.S. Stewart, 1999 *The multi-dimensional stability of weak heat release detonations*. J. Fluid Mech. **382** 109–135.

- **§5(b) PI-Stewart**

Publications (appeared, submitted, in preparation by D. Scott Stewart and students) 2001-2:

(1) A. Kasimov & D. S. Stewart 2001 *Spinning Instability of Gaseous Detonations*, Journal of Fluid Mechanics, accepted March, 2002.

(2) A. Kasimov & D. S. Stewart 2001 *Towards the Miniaturization of Explosive Technology*, Shock Waves, accepted February, 2002.

(3) G. A. Ruderman & D. S. Stewart & Jack Yoh 2001 *A Thermomechanical Model for Energetic Materials with Phase Transformations*, SIAM Journal of Applied Mathemtics, accepted April 2002.

(4) Jack Yoh, D. S. Stewart & G. A. Ruderman 2001 *A Thermomechanical Model for Energetic Materials with Phase Transformations: Analysis of Simple Motions*, SIAM Journal of Applied Mathemtics, accepted April 2002.

Work currently in preparation, supported by this grant

(5) A. Kasimov & D. S. Stewart *The linear stability of nonideal detonation*, in preparation.

Abstract

The linear stability of detonation has been fairly well-studied for a standard model that assumes that the gas obeys an ideal equation of state and with a one-step, depletion rate law with typical Arrhenius kinetics. Recent Short and his collaborators, have focused on extending both the linear and nonlinear stability theory where the one-step Arrehnius kinetics are replaced by more realistic multi-step kinetics. This is an important development.

However, when one considers condensed phase explosives, it is necessary to use non-ideal equation of state (EOS) forms for the constitutive theory so that the models can accurately predict the observed shock properties. Eventually it is important to consider more complex kinetics with non-ideal EOS, but that is *not* the first consideration. Our work here at Illinois, funded in part by other grants from the DOE and the AF through Eglin, AFB, have led us to propose EOS-forms that can predict the experiment shock behavior over a very wide range of conditions that are observed in experiment.

With better EOS forms we have started to carry out linear stability calculations for real condensed phase explosives. We have re-formulation the stability problem and modified some of our existing codes use in our gas phase work. This work, when completed will be the first rational attempt to construct a linear stability theory to non-ideal explosives.

(6) A. Kasimov & D. S. Stewart *Detonation Shock Dynamics in the limit of small heat release*, in preparation.

Abstract

This work will complete A. Kasimov's Ph.D. thesis. He is carrying out a bifurcation analysis of weak-heat release, CJ detonations and we plan to show that the resulting Landau-Stuart equations, thus derived, obtain limiting forms of the Stewart/Yao detonation cell equation. This will essentially complete an analytic theory of cellular detonation first published by us in 1996, and finalize that analysis. It is anticipated that the work will be completed in the Fall of 2002.

Awards

Aslan Kasimov was a second year winner of the UIUC, College of Engineering Mavis Fellowship. This is a highly competitive fellowship and Kasimov is distinguished to win it two years in a row. It carries with it a $5,000 monetary award.

Transitions

Jack Yoh supported by AFRL (primarily Eglin AFB, Munitions Directorate) graduated in December 2001. His Ph. D. thesis was entitled

(7) A. Kasimov & D. S. Stewart *Thermomechanical and numerical modeling of energetic materials and multi-material impact*, , University of Illinois, College of Engineering, Theoretical and Applied Mechanics, Dec. 2001, Ph. D. advisor D. S.

Jack recently has been hired by Lawrence Livermore National Laboratory as a Technical Staff Member. Jin Yao, formerly here at Illinios, also recently was hired by Lawrence Livermore National Laboratory as a Technical Staff Member, in B Division.

Other related activity indirectly supported by this grant

(8) Jack Yoh & D. S. Stewart *High-resolution, numerical modeling of energetic and inert materials at large deformation rates*, submitted to Combustion Theory and Modeling

Abstract

This paper describes the methodology used to build a high-resolution, multi-material hydrocode that is formulated to be third order in time and fourth order in space. The hydrocode is suitable for simulating high-speed impact and interaction of energetic and inert materials. Energetic materials are modeled by the reactive Euler equations. The

inert materials can be modeled by either the Euler equations or by constitutive laws that can describe metals. Level set functions are used to track the motion of multi-material interfaces between fluids, solids and free surfaces (or voids). A technique is used to extrapolate material states into extended ghost node regions to enforce boundary conditions. A standard pressure update is used near the material/material interfaces. The algorithms are verified with a collection of standard test problems, and the function of the code is demonstrated with a series of representative applications that include: copper rod impact, explosive rate-stick, explosive welding, and the impact of a copper plate by a cylindrical detonation.

We are very excited about this new simulation capability and plan to use it in our continued work on miniaturization of explosive technology. Our new code is currently named GIBBS2D. Our plans include integrated, theory simulation and experiment.

(9) D. S. Stewart, Ron Adrian & S. Chaieb *Ongoing developments in miniaturization of explosive technology at UIUC.*

Our efforts on miniaturization have accelerated. Los Alamos National Laboratory is going to sponsor Ron Adrian and Scott Stewart to develop a micro-doppler-global velocimetry system to look at the surfaces of micro-sized exploding foils and other elements of detonation initiation systems. The main load of the experimental work will be carried out by Adrian, but Stewart will be providing computational simulation support concurrently, using the new code GIBBS2D, described above.

Porous Silicon

In addition we have a new colleague, S. Chaieb, assistant Prof. of Theoretical and Applied Mechanics, who has been working with Adrian and Stewart. Chaieb has independently been creating the porous silicon for other nano-particle studies and has agreed to work with us. Our interest in this accelerated with Dr. Arje Nachman, brought a recent the Science News article on treated porous silicon to the attention of D. S. Stewart. Stewart saw this system as an accessible and interesting one that could be a candidate for use with explosive films or energetic film substrates. Recently 4/25/02 Chaieb has taken picture of nitrated surfaces of porous silicon hit with pulsed laser in Ron Adrian's laboratory.

This activity will continue and the some of those elements that are part of mathematical modeling will likely be included in any follow on proposal to AFOSR (Dr. Nachman). We are very excited about these recent developments and believe it to be an area of growing national interest.